

Comment on ‘On the Luttinger theorem concerning the number of particles in the ground states of systems of interacting fermions’, arXiv:0711.0952v1, by B. Farid

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In his preprint [1], arXiv:0711.0952v1, Behnam Farid argues that the Luttinger theorem is valid not only for a metal but also for a Mott insulator if the chemical potential is calculated by taking the limit of vanishing temperature at fixed particle density. In contrast, we have found in our recent paper [2] on the basis of a controlled strong coupling expansion that the Luttinger theorem is violated in this limit for a particle-hole asymmetric two-band Mott insulator. In an extensive discussion of our result Farid argues that an arbitrarily weak breaking of particle-hole symmetry leads to a destruction of the Mott insulating state at half filling. In this comment we point out that this is not correct.

In a recent paper [2], we have shown that in a certain two-band Hubbard model in its Mott insulating phase the Luttinger theorem (in the variant given below) is not valid for a range of chemical potentials. The Luttinger theorem

$$n = 2 \sum_{\alpha} \int_{G_{\alpha}(\mathbf{p}, \omega=0) > 0} \frac{d^3 \vec{p}}{(2\pi)^3} \quad (1)$$

relates the density of particles, n , to a volume in momentum space where the Greens function at $\omega = 0$ is positive. Here α is a band index. In the case of a Mott insulator, the Greens function changes its sign without having a pole at the so-called Luttinger surface, see references in [1] and [2].

It is very easy [2] to convince oneself that the right-hand side of Eq. (1) depends on the chemical potential μ when μ is varied *within* the gap of a Mott insulator [as $G(\mathbf{p}, \omega, \mu) = G(\mathbf{p}, \omega + \mu)$]. In contrast, the left-hand side is independent of μ at $T = 0$ for any value of μ within the gap. Therefore there is typically only a single value of the chemical potential, $\mu = \mu_L$, within the gap where (1) is valid (as shown explicitly in Ref. [2]).

Farid [1] agrees that the Luttinger theorem is not valid for a range of chemical potentials but argues that no such problem can arise when the chemical potential is calculated in the limit $T \rightarrow 0$ at fixed particle density n , $\mu_n = \lim_{T \rightarrow 0} \mu(n, T)$ (Farid uses the notation $\mu_{\infty} = \mu_n$).

In contrast, we obtained in Ref. [2] within a controlled strong coupling expansion that even in this limit, the Luttinger theorem is not valid for a generic particle-hole asymmetric situation, $\mu_n \neq \mu_L$. We used that μ_n is located in the middle of the gap such that the activation energies of many-particle eigenstates with particle number $N - 1$ and $N + 1$ are identical. A calculation of μ_n (and μ_L) to linear order in $1/U$ turns out to be sufficient [2] to construct a counter example to the Luttinger theorem for $\mu = \mu_n$.

On the pages 58 to 86 of his preprint Farid discusses these questions, analyzes our result and comes to the conclusion that we determined μ_n in an incorrect way

when taking the limit of zero temperature at fixed particle density. His argument is based on a surprising result of his calculations: he claims [3] that an arbitrarily small breaking of particle-hole symmetry transforms the half-filled Mott insulator into a metal, or, equivalently, that the particle-hole asymmetric system is not half-filled if the chemical potential is located within the gap! In our opinion, this is obviously wrong. For example, it contradicts the observation that small perturbations have no effects in systems with a finite gap (in the two-band Mott insulator under consideration both the charge and the spin gap are finite). In the appendix we sketch the formal argument which can be used to prove this.

But it is also useful to check how the surprising result is obtained in Ref. [1] that the Mott insulating state is not half filled. In Eq. (6.50) the electronic density, n , of the Mott insulating phase is calculated by using formula (6.36) [or, equivalently (6.43)] for the Greens function which is obviously only valid up to order t/U . In the absence of particle-hole symmetry, Farid argues that the deviation from half-filling, $n - 1$, is finite at $T = 0$ and of order $(t/U)^3$ (see sentence below Eq. (6.59)). It is, however, not possible to calculate a quantity to order $(t/U)^3$ based on an approximate formula which is valid only up to order t/U .

The wrong interpretation of this calculation seems to be the reason, why Farid disagrees with our finding [2] that the Luttinger theorem is not valid for $\mu = \mu_n$.

I would like to thank B. Farid for discussions which helped me to understand his point of view.

Appendix: Particle density of a Mott insulator

In this appendix we briefly sketch a formal argument which can be used to proof that a Mott insulator remains half-filled at $T = 0$ in the presence of weak particle-hole asymmetry. Here we consider the two-band Mott insulator defined in Ref. [2] which has a unique ground state and a gap not only in the charge sector but also in the spin sector. We start with a particle-hole symmetric

model with N_0 sites. Due to the particle-hole symmetry, the system is half-filled, $N = \langle \hat{N} \rangle = N_0$. Now, we track the evolution of the ground state when particle-hole symmetry is broken, e.g. by switching on a weak next-nearest neighbor hopping t' . As $[H, \hat{N}] = 0$, the ground state is always an eigenstate of \hat{N} , and as \hat{N} has a discrete spectrum, the groundstate remains exactly half-filled as long as there is no level-crossing. As the gap of the Mott insulator is finite in the thermodynamic limit, no such level crossing can occur for small t' .

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- [1] B. Farid, preprint arXiv:0711.0952v1 (2007).
 - [2] A. Rosch, Eur. Phys. J. B **59**, 495 (2007).
 - [3] e.g. page 57 of [1]: “*We shall rigorously demonstrate that irrespective of how minute the deviation of $D(-\omega)$ from $D(\omega)$ may be, such deviation transforms the insulating GS ... into a metallic GS*”, see also Eq. (6.50), the statements above Eq. (6.60) or the concluding remarks on p. 86.